Evolution of the Fabric Tensor in Amorphous Silica: via Molecular Dynamics Simulations

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AFM (Atomic Force Microscopy) experiments and MD (Molecular Dynamics) simulations have revealed a process zone (PZ) near the crack tip in amorphous silica (a-SiO_2). Within this process zone pores nucleate and coalesce with one another up to 20 nm ahead of the crack tip [1-4]. After which the cavities merge with the advancing crack to cause mechanical failure. Similarly, when a-SiO_2 sample is nanoindented one finds permanent damage under the indenter in the form of densified silica [6].
To shed light on the origin of irreversible deformation in amorphous media where the notion of dislocations is irrelevant, MD simulations have been performed in a-SiO_2 systems which are subjected to (1) a cyclic loading and unloading of the hydrostatic pressure and (2) a shearing force at room temperature. In particular, the so-called fabric tensor commonly used in granular physics is computed and allows to evidence anisotropy setting in the structure silica [7].

References

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